# Hemanta Bhattarai

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Computational Physicist with 10+ years of experience in programming and scientific computing. Proficient in mathematical modeling using available data. Expert in simulating the systems with the developed model, analyzing the outcome from simulation, and conclude the results. Solid understanding of machine learning algorithms and data analysis. Equipped with strong analytical and problem-solving skills

## Education

**University of Notre Dame** — Notre Dame, IN
Ph.D., Physics — 2015–Current

## Experience

**University of Notre Dame** — Notre Dame, IN
Research Assistant — 2015–Current

- Developed a mathematical model for metals, (DR-EAM), and parameterized model parameters to capture most metals' features. Performed molecular dynamics simulations of metals and alloys to test the validity of the model. Used the developed model to predict the different properties of metals and alloys.
- Modeled an energy surface for metal and water interaction and simulated the metal-water interface using the model. Studied transport properties at the interface using non-equilibrium molecular dynamics simulations and analyzed the orientation of water at the metal surface.
- Re-tuned DR-EAM parameters for Oxygen (DR-EAM.v2) to study the oxides' formation and growth on the metal surface. Developed a new mixing rule for the intermolecular potentials of metals and oxygen in oxides.
- Developed different modules in OpenMD, (http://openmd.org), a molecular dynamics software developed and maintained by Gezelter's Lab (http://gezelterlab.org). Implemented molecular dynamics algorithms and analysis scripts in C++, python, and bash. Trained new graduate students to use OpenMD.

Teaching Assistant — 2015–2017

- Collaborated with instructors in test administration and assignment grading for graduate and undergraduate.
- Planned physics labs and organized help sessions for students.

## Data Science Courses

- **University Courses**: Advanced Machine Learning, Data Science, Computational and Data Analysis for Physics, Introduction to Network Science.
- **UDEMY:** CUDA Programming Masterclass, Master SQL for Data Science, Deep Learning A-Z$^{TM}$: Hands On ANN, Advanced C++ Training Course, Python Beyond The Basics - Object-Oriented Programming

## Skills

- **Programming:** Python, C++, Matlab, Bash, Linux
- **Packages:** CUDA, Pandas, Scikit-learn, Keras, Git, GDB
- **Simulation Techniques:** Molecular Dynamics, GAMMES, VASP
- **Machine Learning Algorithms:** Supervised Learning (Linear Regression, SVM, KNN, Decision Trees), Unsupervised Learning, Deep Learning

## Publications

1. **H. Bhattarai**, K. E. Newman, and J. D. Gezelter,"The Role of Polarizability in the Interfacial Thermal Conductance at the Gold-Water Interface", J. Chem. Phys., 153, 204703(2020).

2. **H. Bhattarai**, K. E. Newman, and J. D. Gezelter, "Polarizable potentials for metals: The density readjusting embedded atom method (DR-EAM)", Phys. Rev. B, 99, 094106(2019).

3. B. Aryal, **H. Bhattarai**, S. Dhakal, C. Rajbahak, W. Saurer,"Monthly Notice of the Royal Astronomical Society", 434(3), 1939(2013).